$PM_{2.5}$ and Ultrafine PM Chemical Transport Modeling

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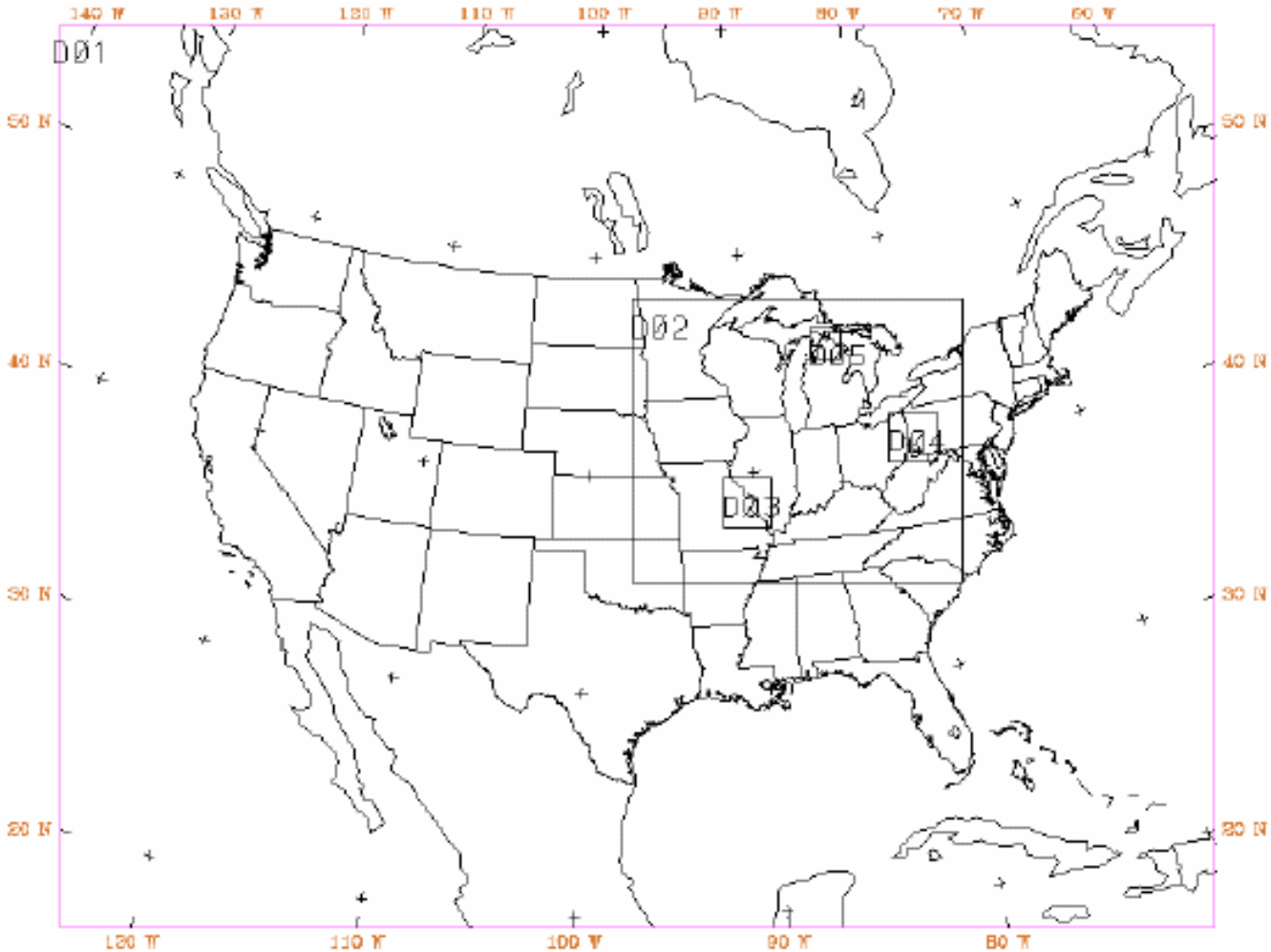
Overview of Project

- Funded by DOE/NETL with some additional support by LADCO
- Collaboration with ENVIRON (Greg Yarwood and Ralph Morris), LADCO, and the St. Louis Supersite.
- Modeling tools
  - PMCAMx
  - Aerosol thermodynamics models (GFEMN, ISORROPIA)
  - Aerosol dynamics models

Modeling Domain for PMCAMx



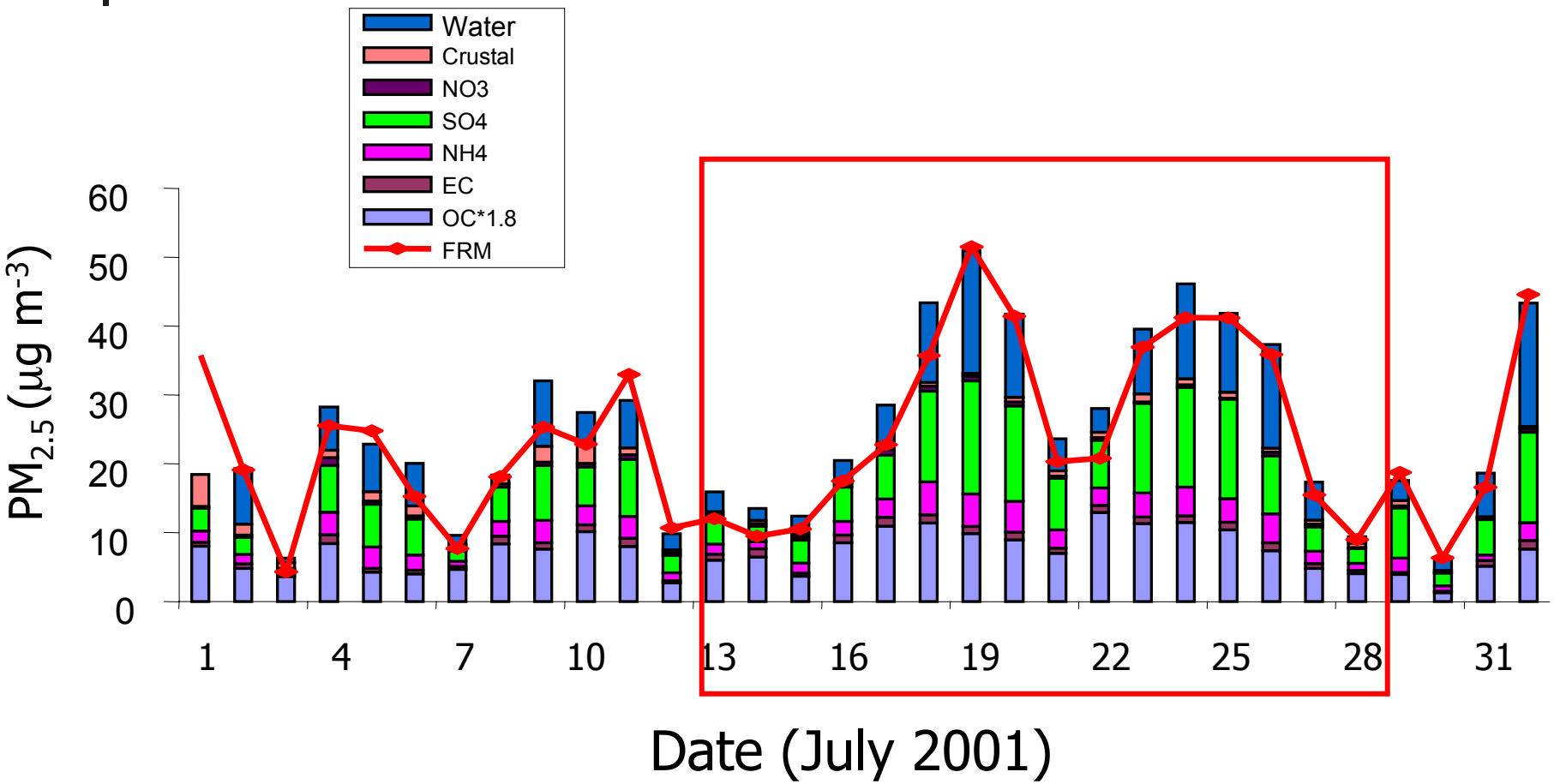
Outer domain
36x36 km

Middle domain
12x12 km

Inner domains
4x4 km

1.5 million computational cells

Simulation Period (July 2001-ESP01)



Significant secondary organic aerosol formation in the 2nd half of July.

Objectives

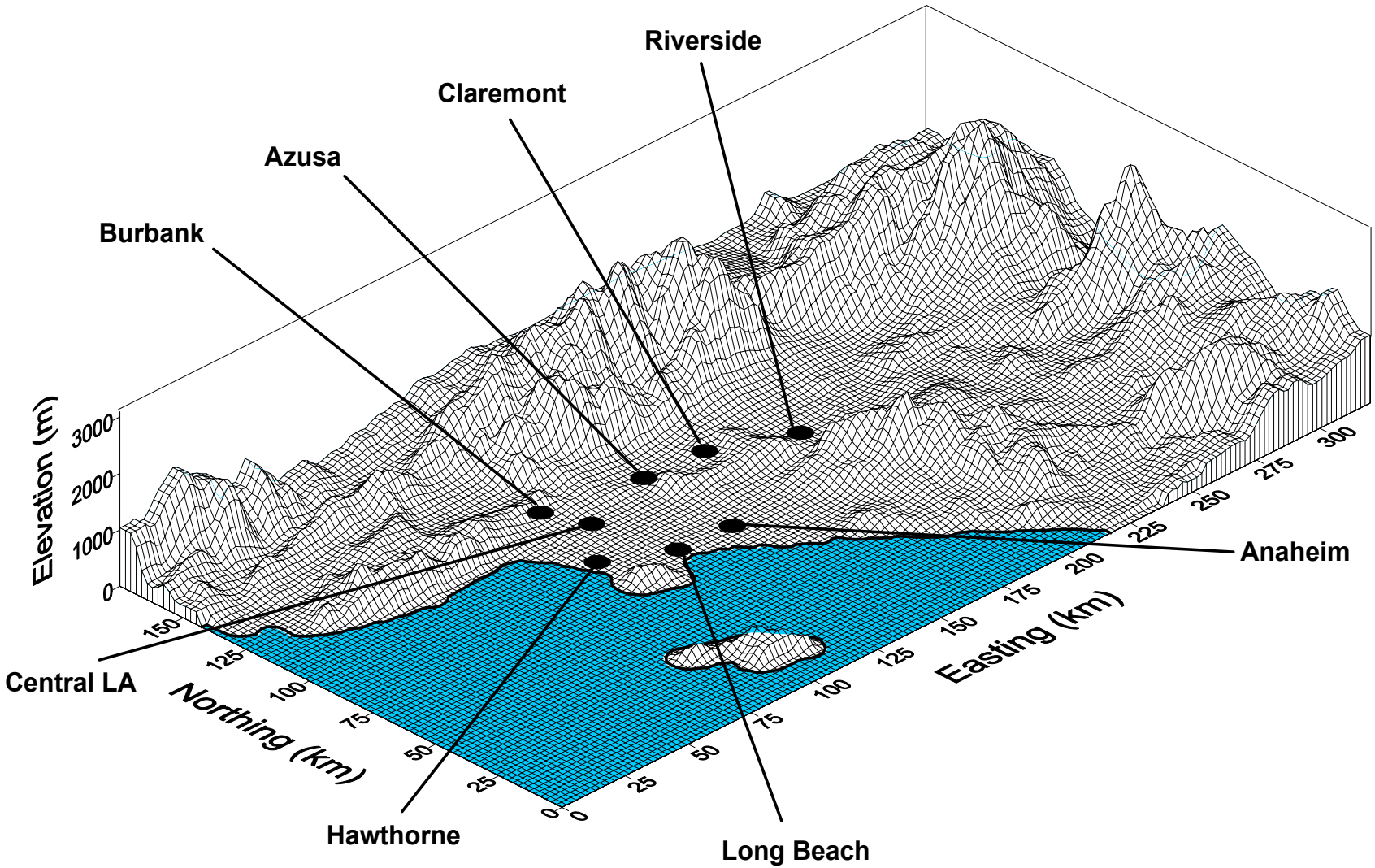
- Evaluation of our understanding of the
  - Formation (sulfate, nitrate, SOA)
  - Emissions (organic PM, dust, industrial emissions)
  - Long range transport
  - Removal (rain, dry deposition)

  of fine PM and its components
- Derivation of source-receptor relationships
  - Contribution of sources
  - Responses to changes in emissions

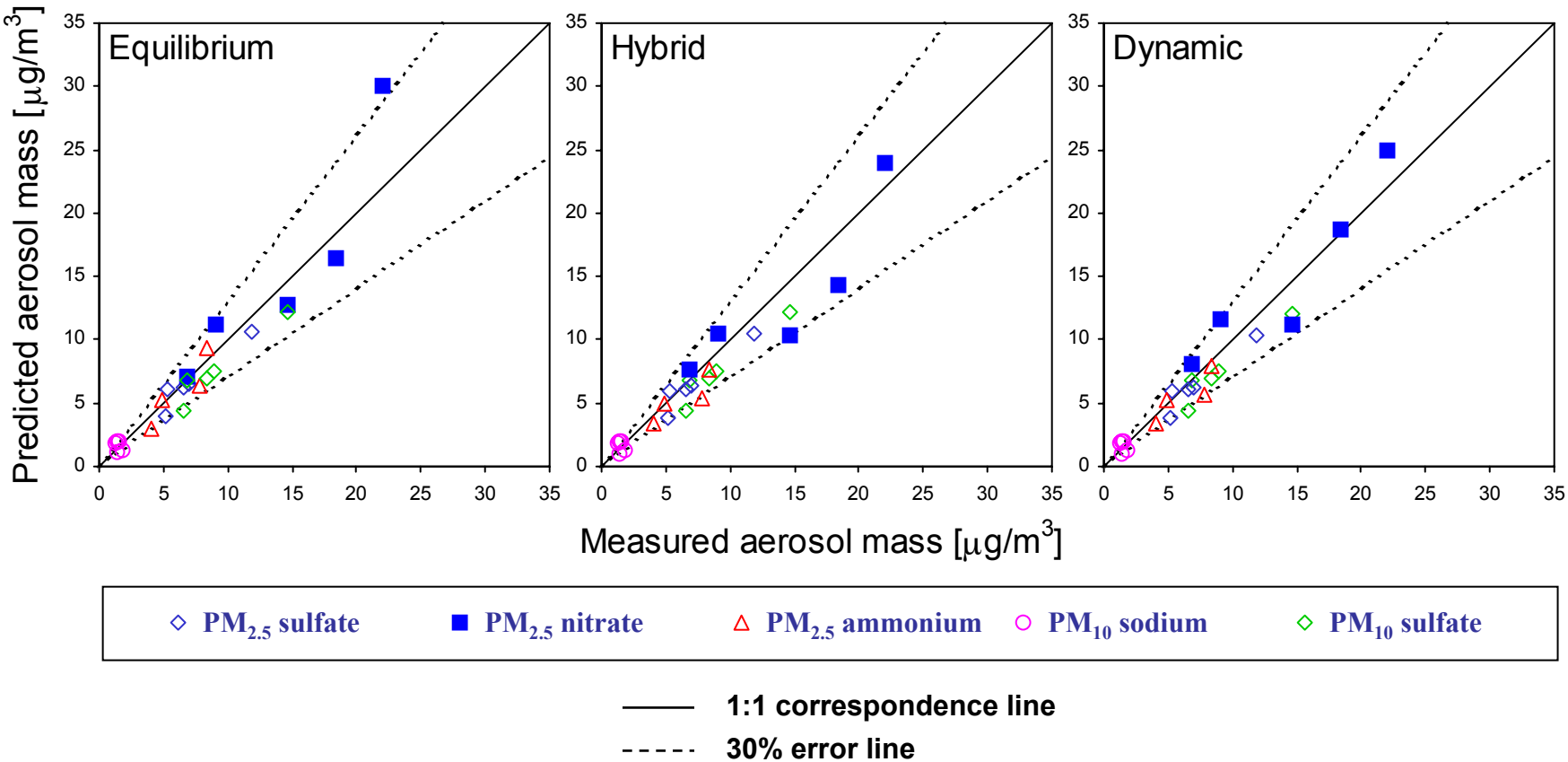
Some features of the CMU Modules

- Aerosol Module (Koo et al., AS&T 2002)
  - User-selected size resolution (sectional model)
  - Equilibrium or Dynamic or Hybrid approach
  - Fast and quite accurate (runs on a PC)
  - Comprehensive SOA module (30 SOA species) including interactions with water and inorganics
- Aqueous-Phase Chemistry Module (Fahey et al., AE, 2002)
  - Variable Size Resolution Model (chooses the cloud droplet resolution for chemical calculations at each step)
- The 2001 versions of the modules have been recently added to CMAQ by Pun et al. (2003)

PMCAMx Testing (Southern California)

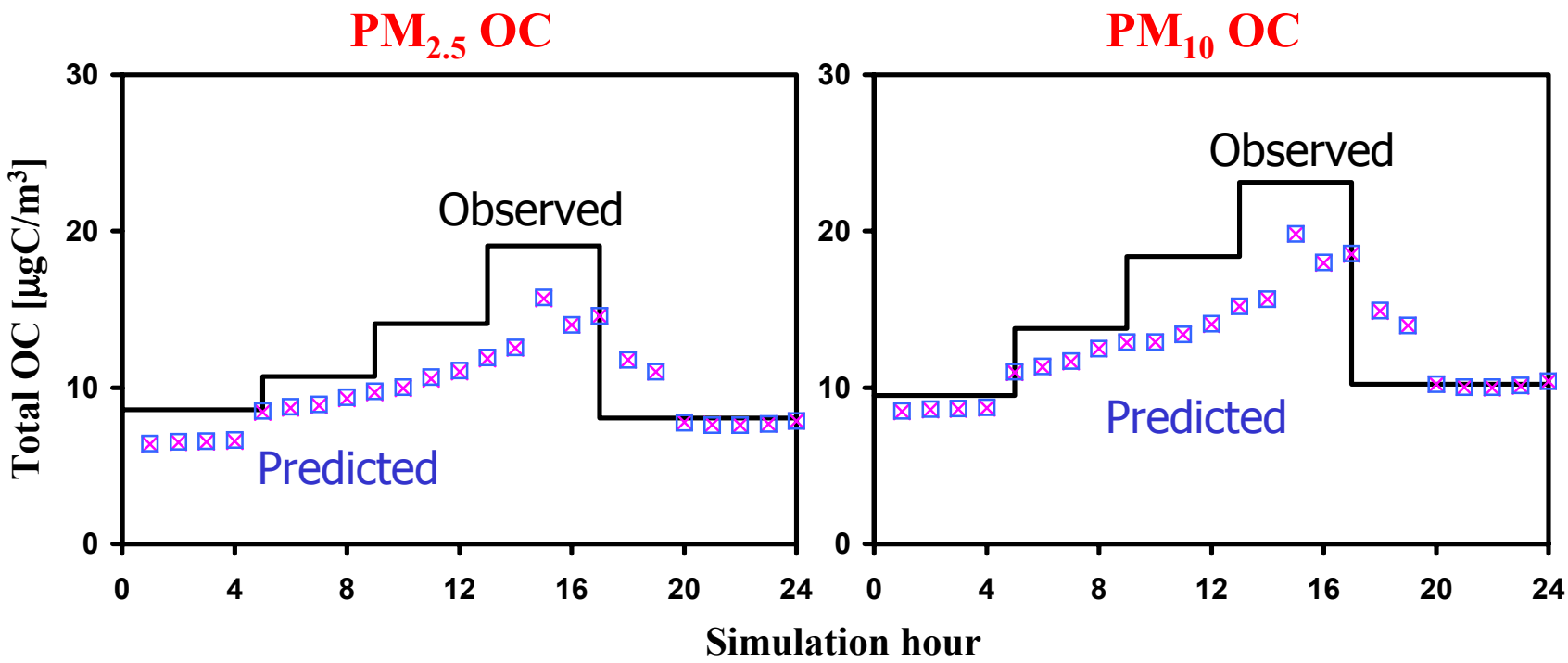


Predicted and Observed 4-6 hr Average Aerosol Mass (Claremont, CA August 28, 1987)



Dynamic Model Evaluation

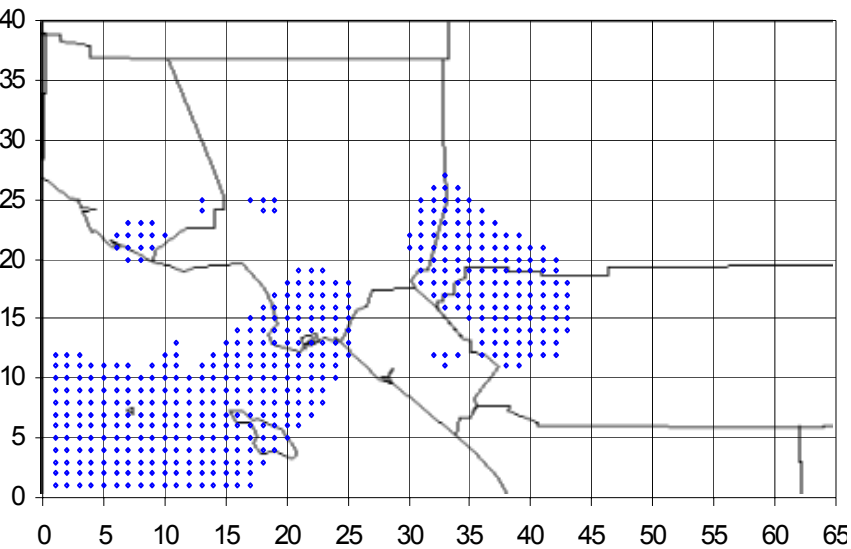
SCAQS episode: Claremont, 28 August 1987



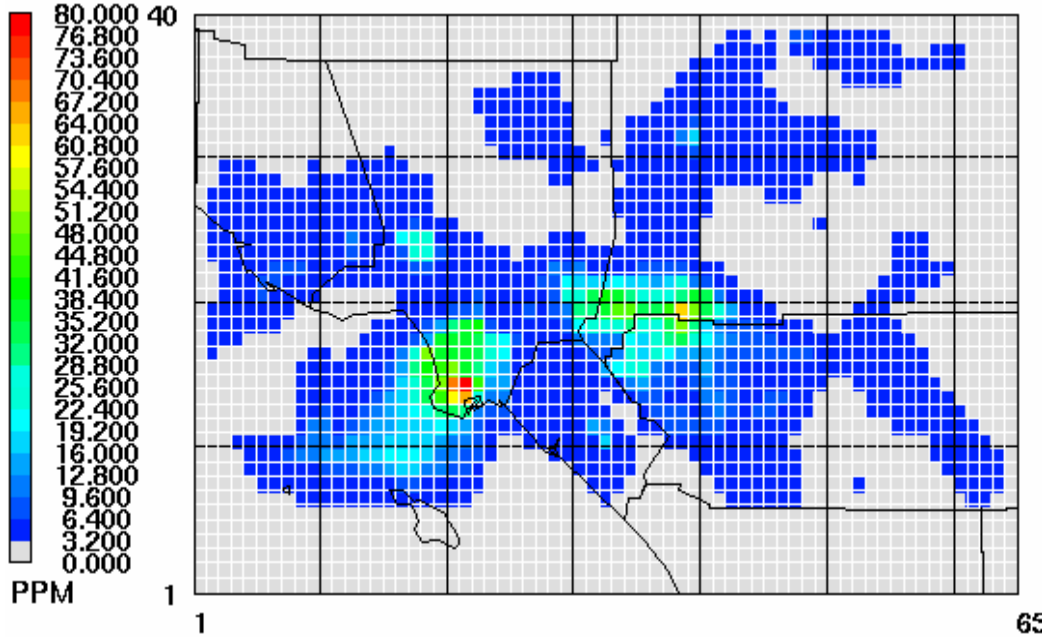
SCAB Fog Episode (October 1995)

October 17, 7:00

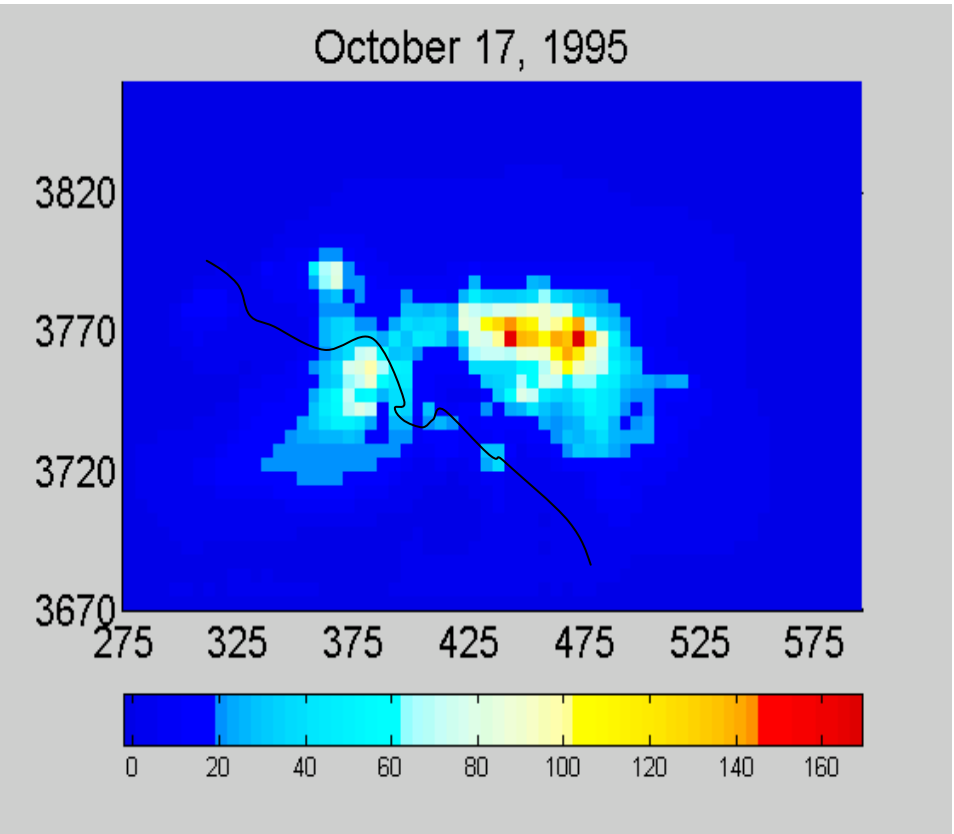
Fog Cover

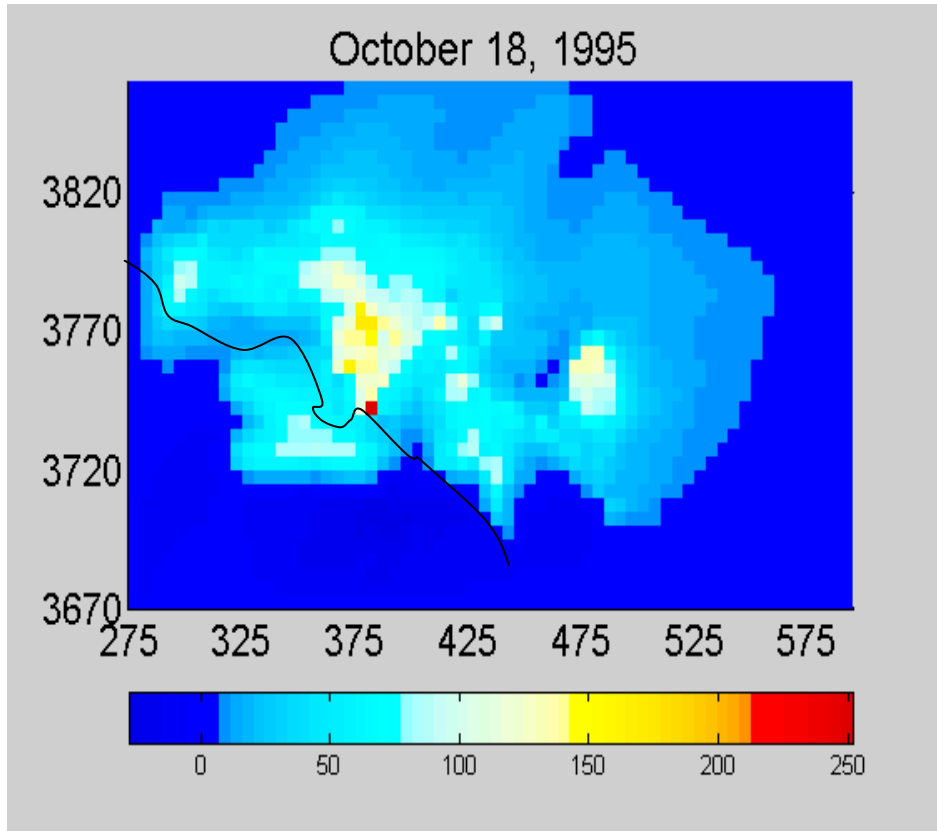


Sulfate Concentration

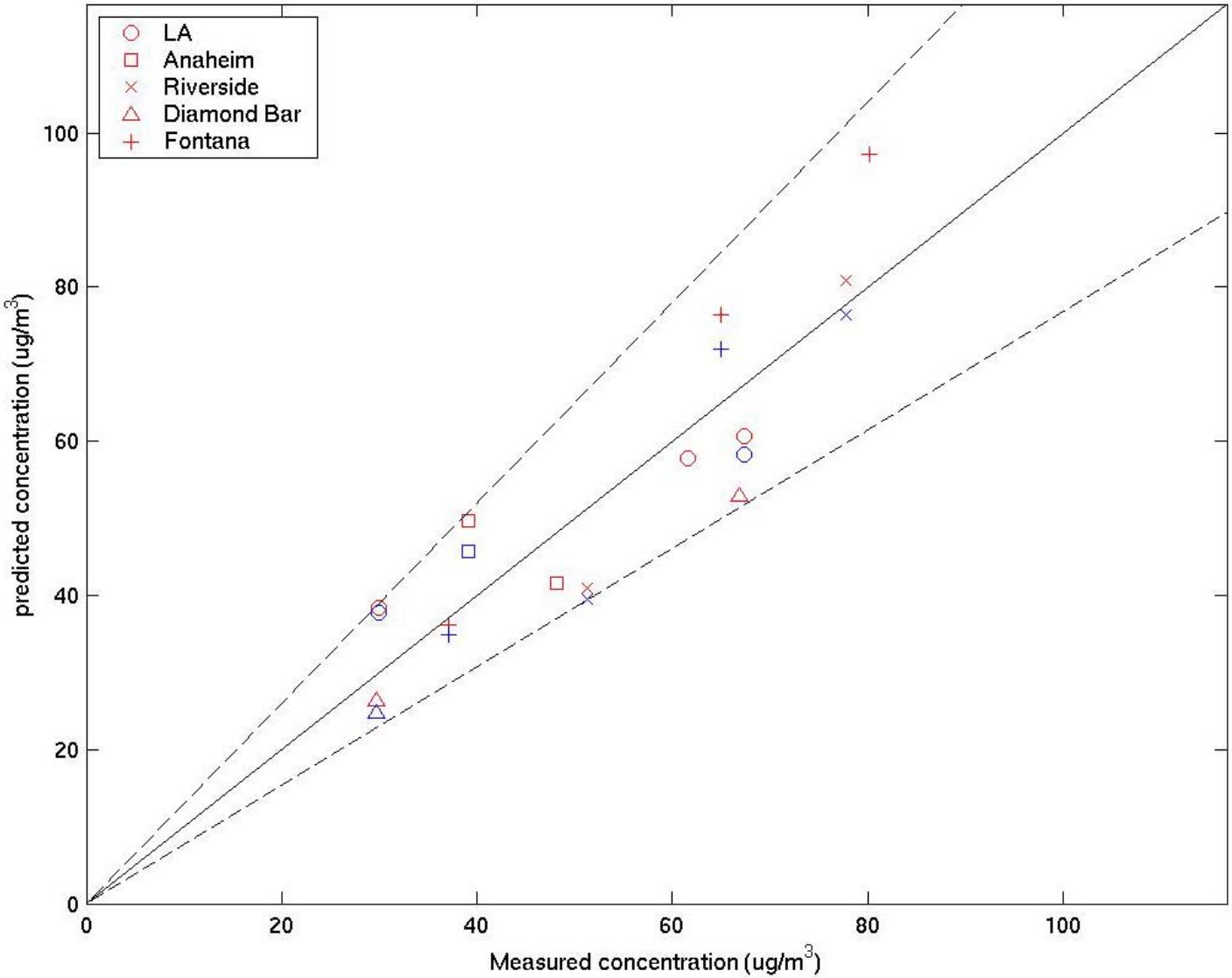


% Sulfate Increase with the Addition of Aqueous-Phase Chemistry

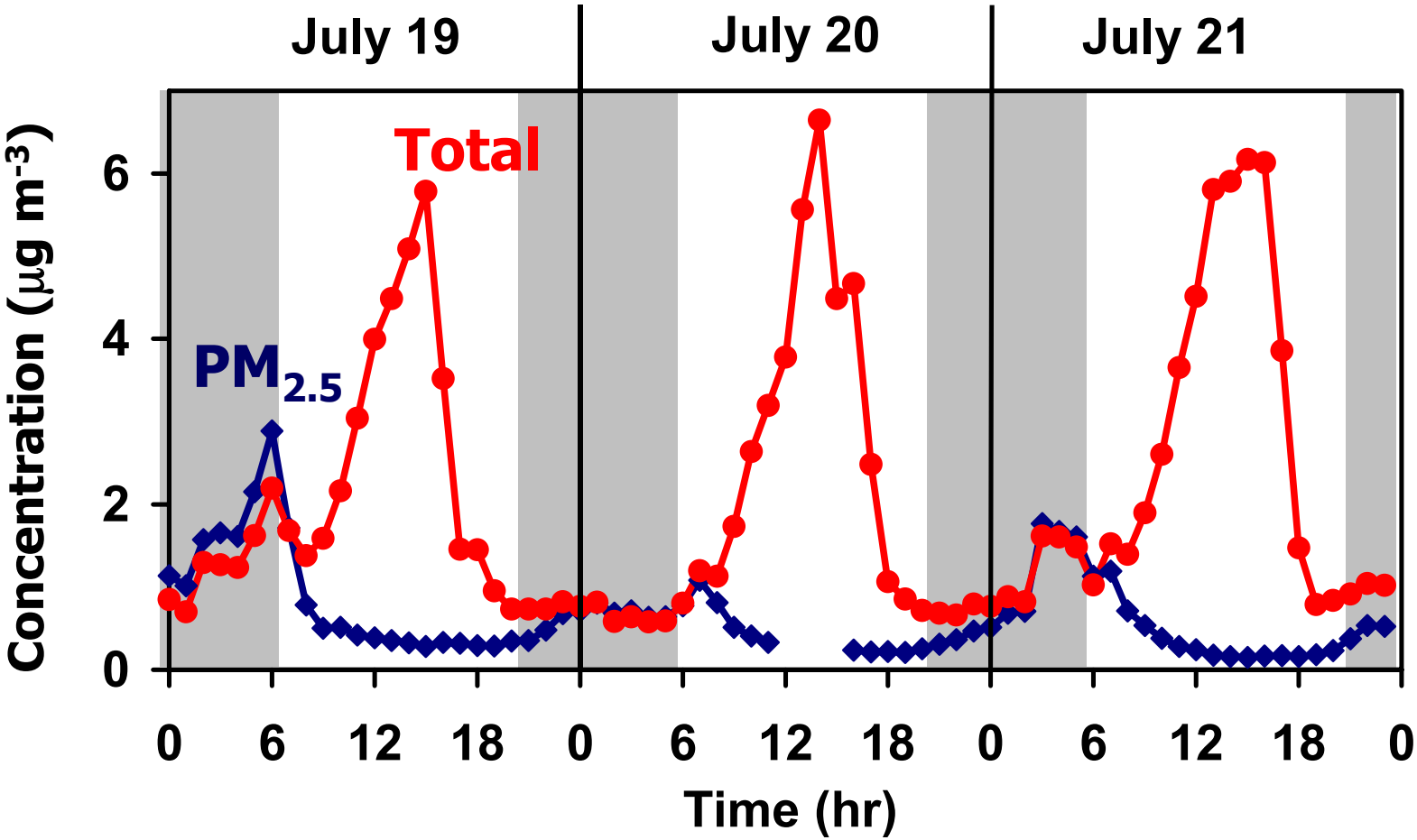




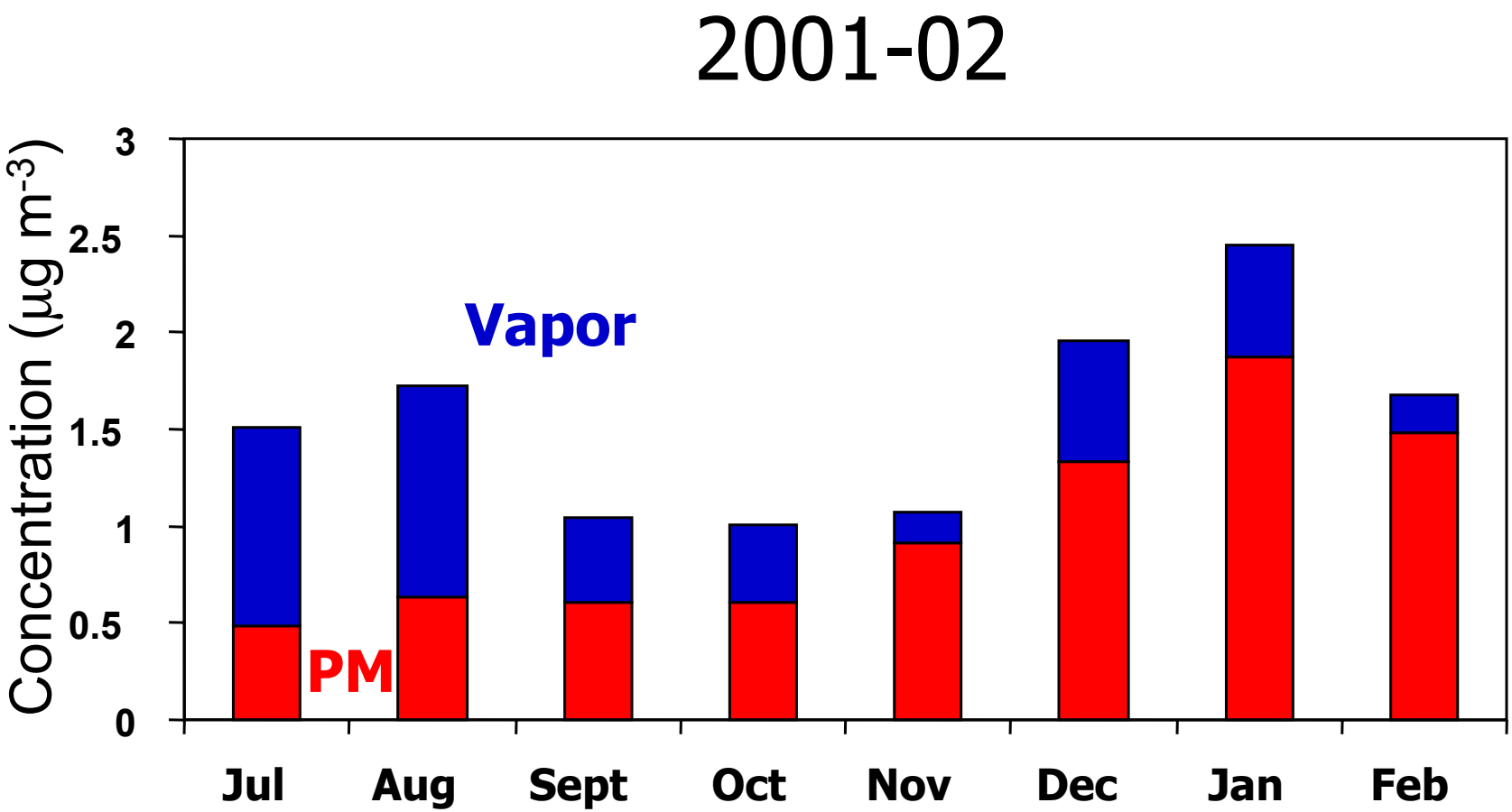
$PM_{2.5}$ Mass Predictions (October 1995)



Partitioning of $PM_{2.5}$ nitrate

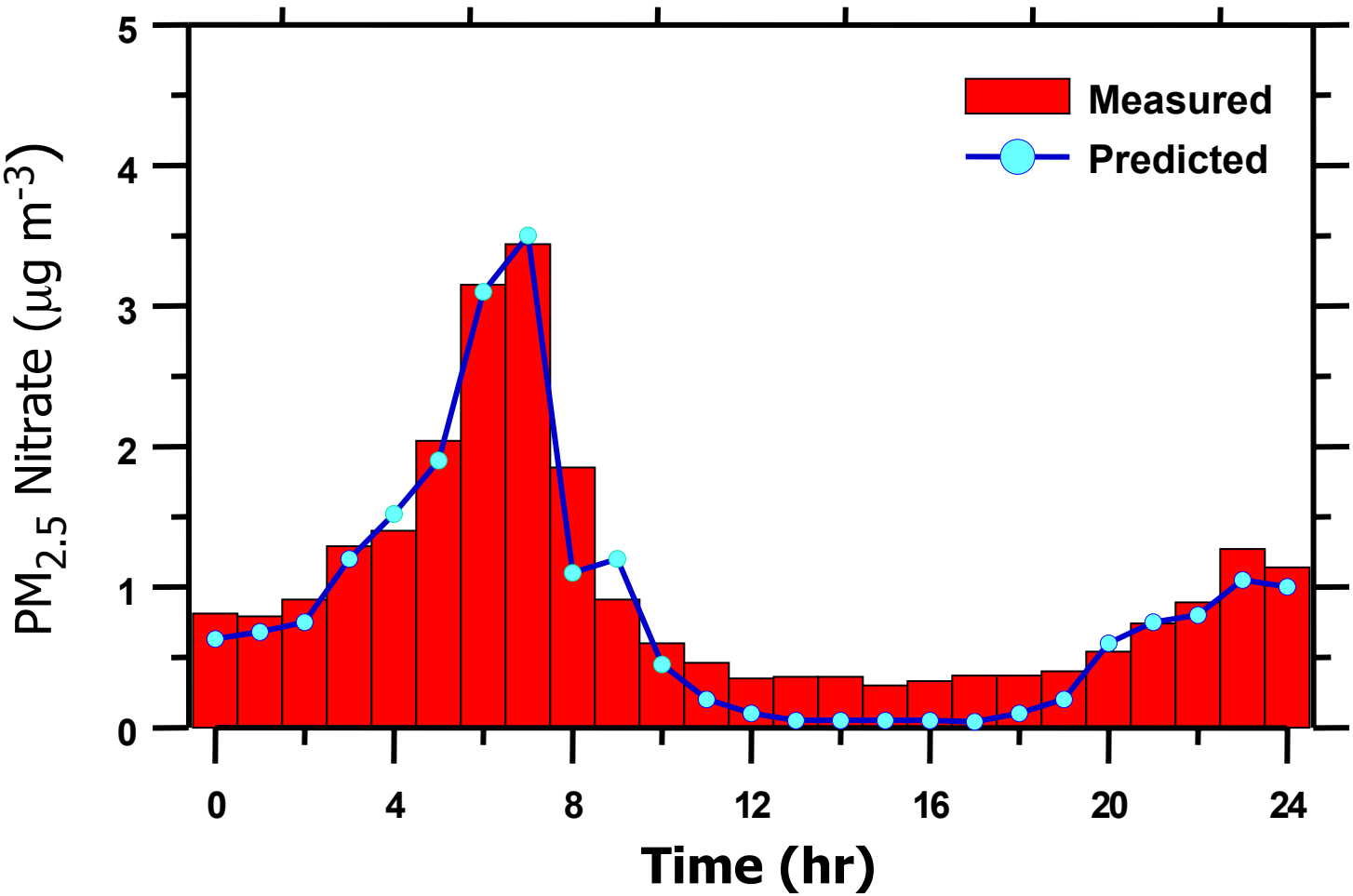


Availability of Nitric Acid and Nitrate

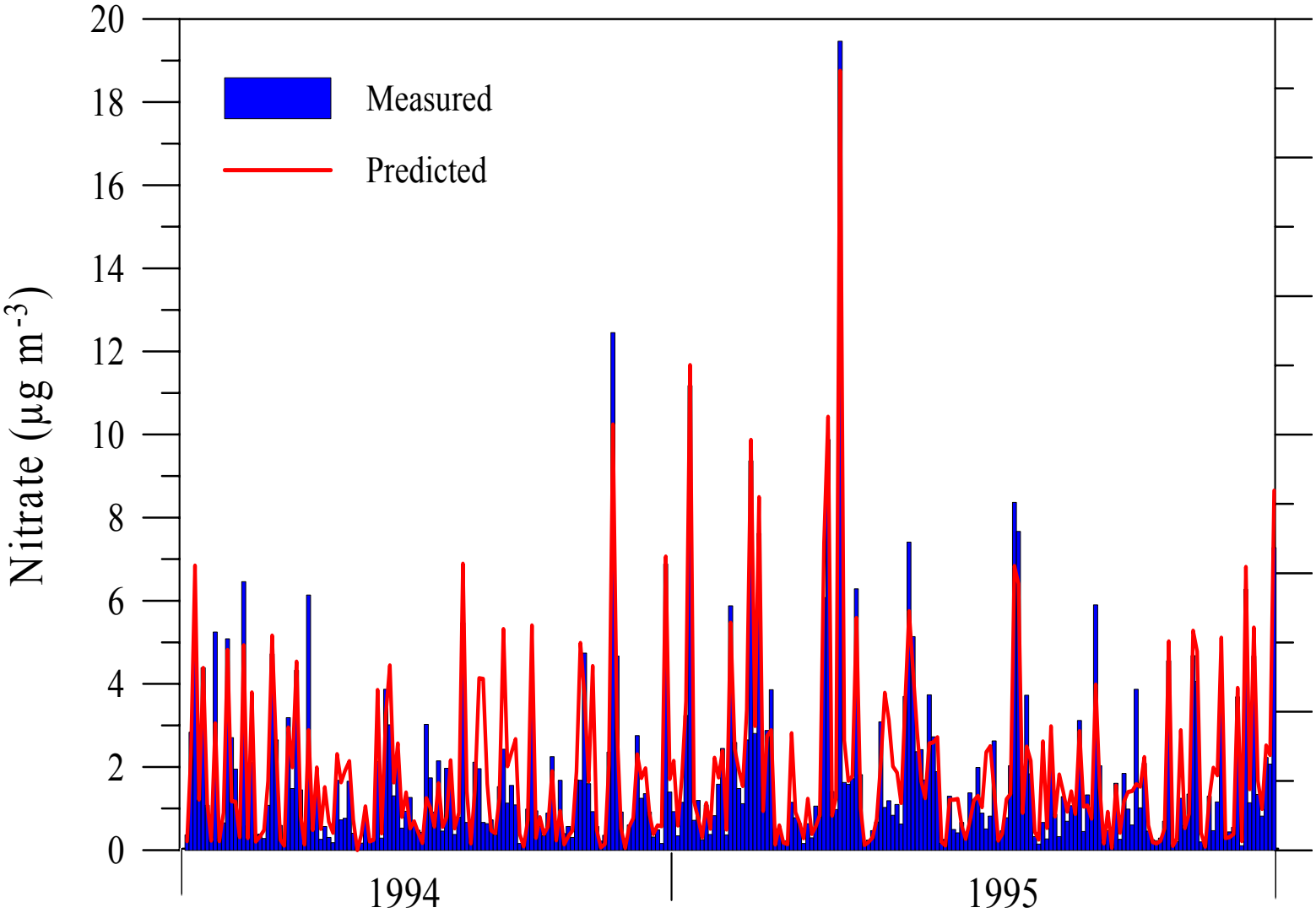


GFEMN Evaluation: Nitrate Partitioning

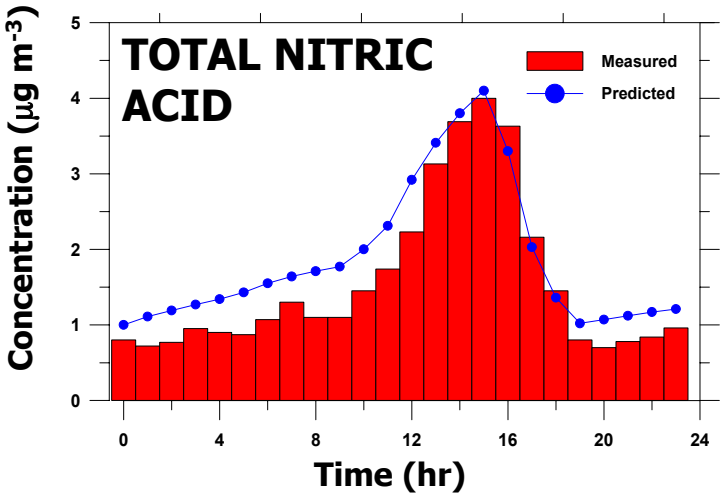
(July 19, 2001)

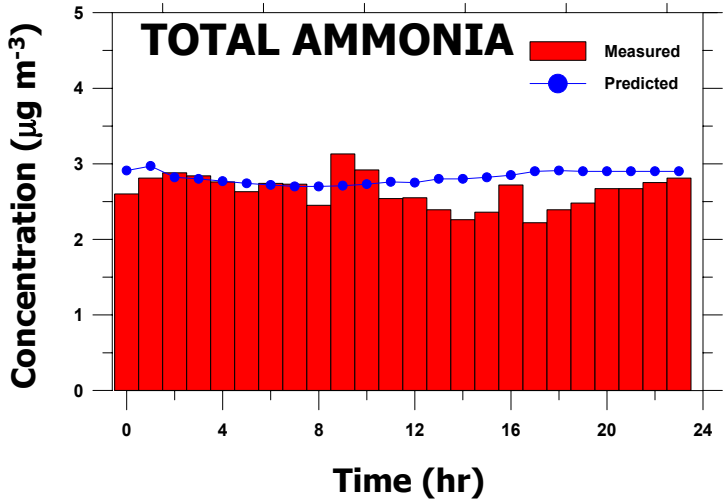


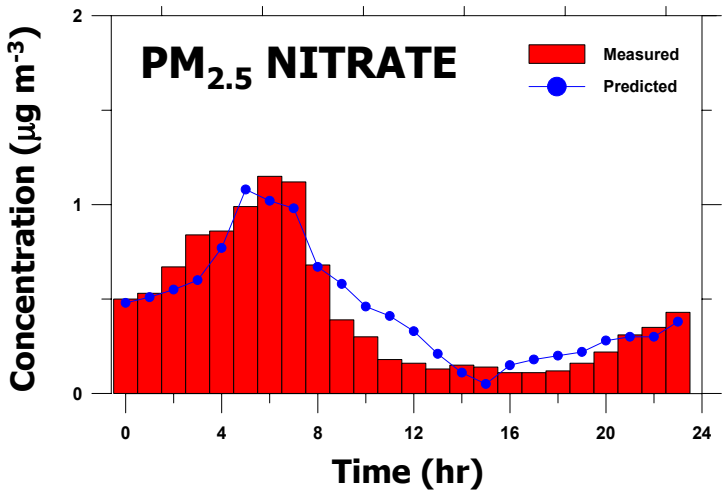
GFEMN Evaluation (Hamilton, Canada)



Evaluation of Box Model

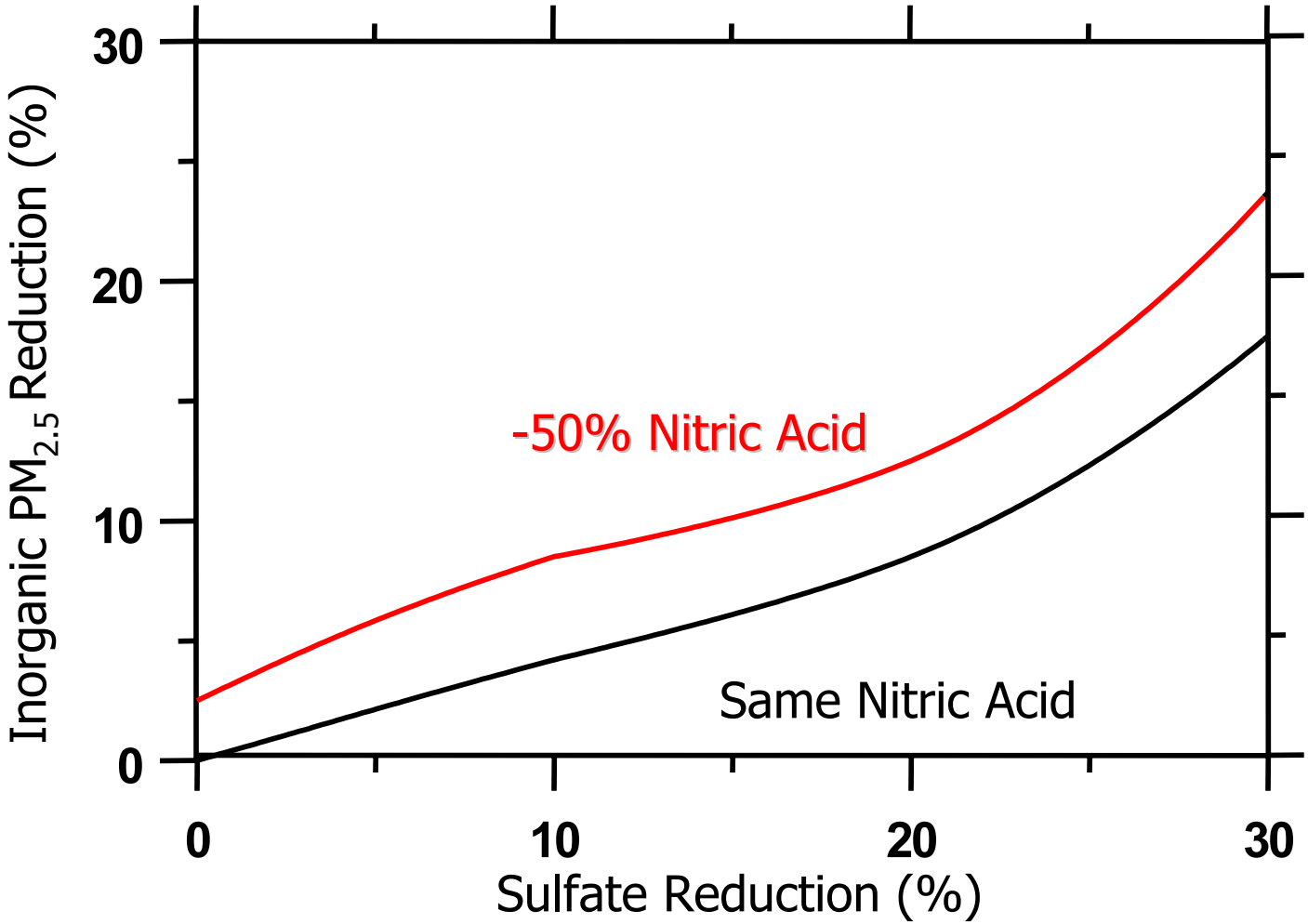




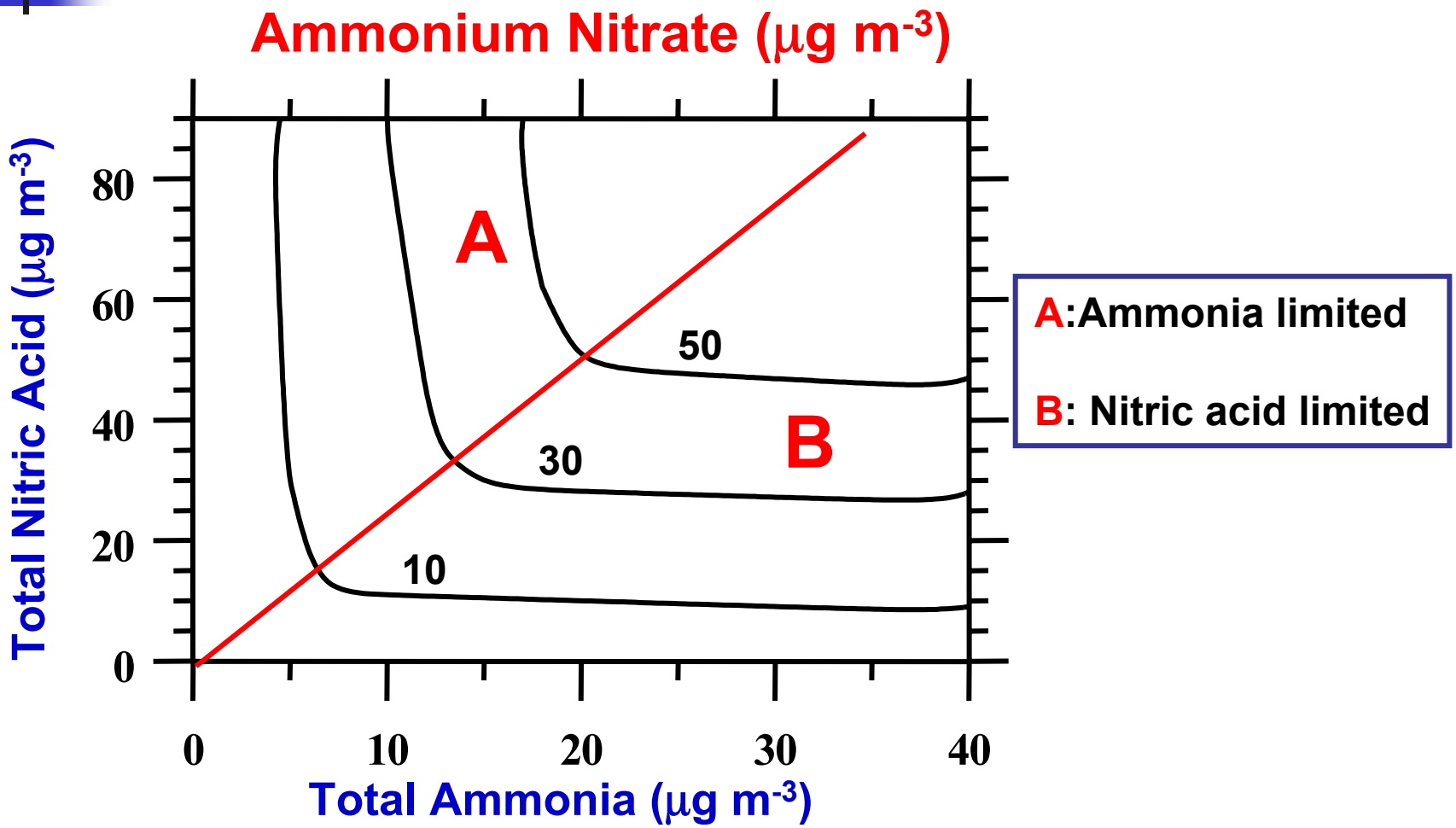


PITTSBURGH
July 2001

Reductions of Sulfuric and Nitric Acid (Pittsburgh, July 2001)

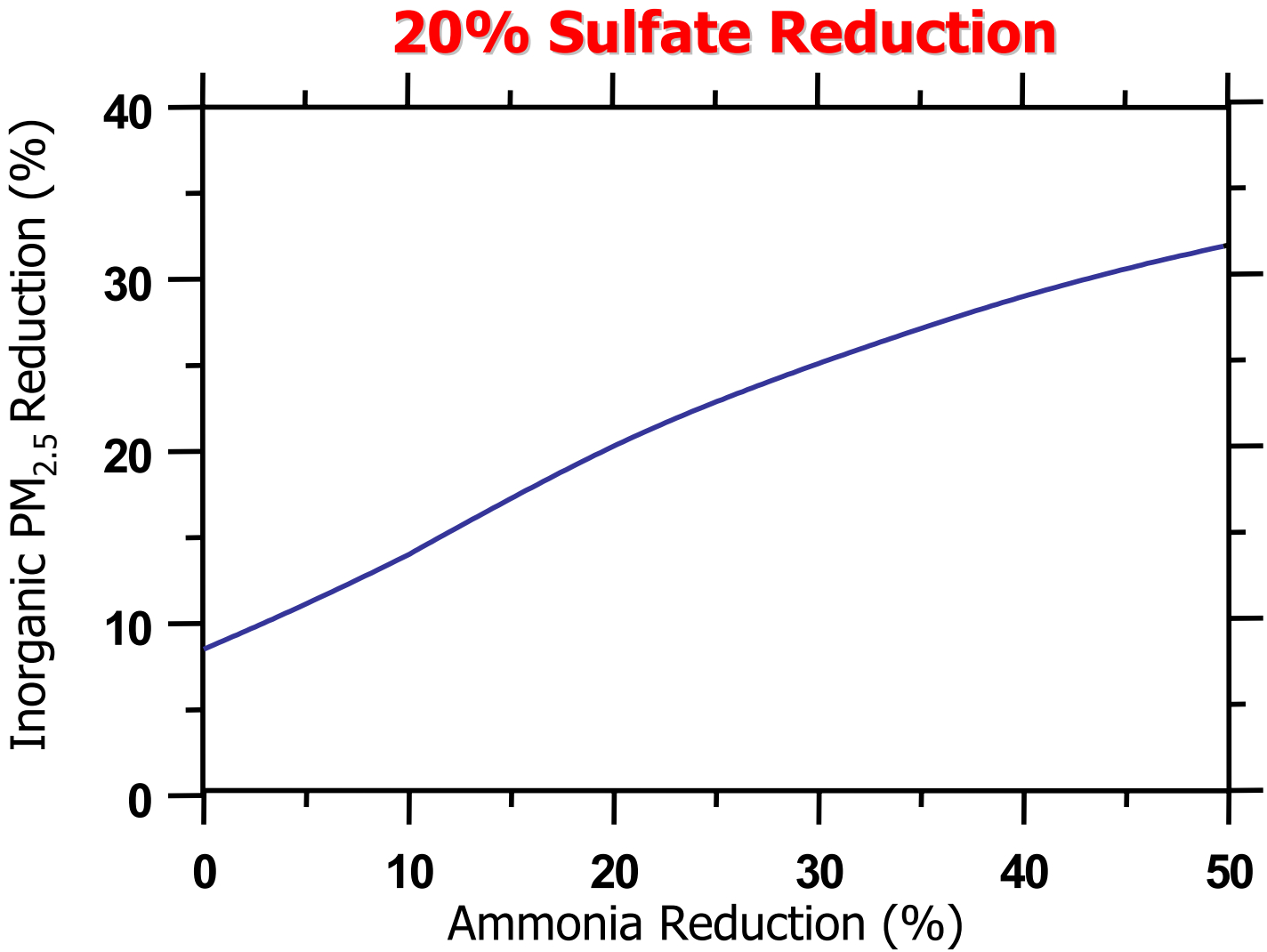


Limiting Reactant: Ammonia or Nitric Acid?

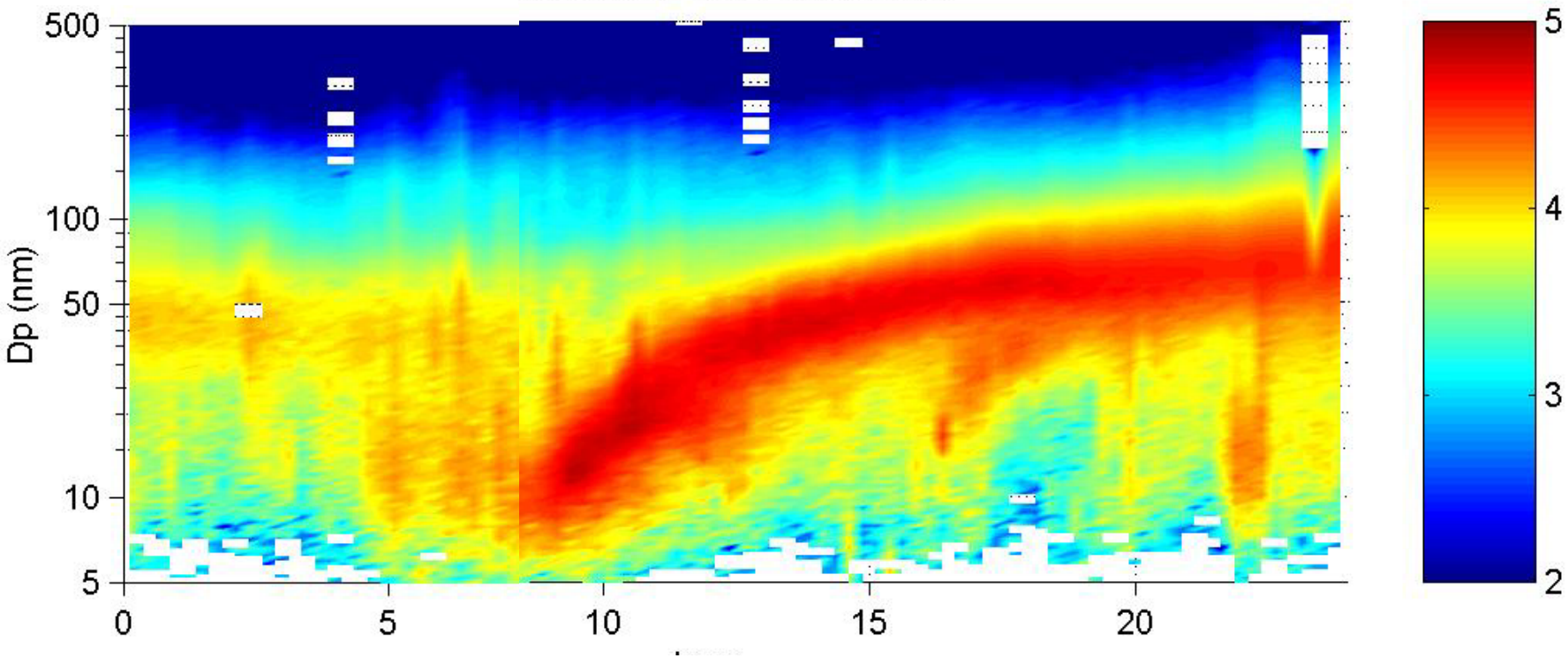


Reductions in Ammonia

(July 2001)

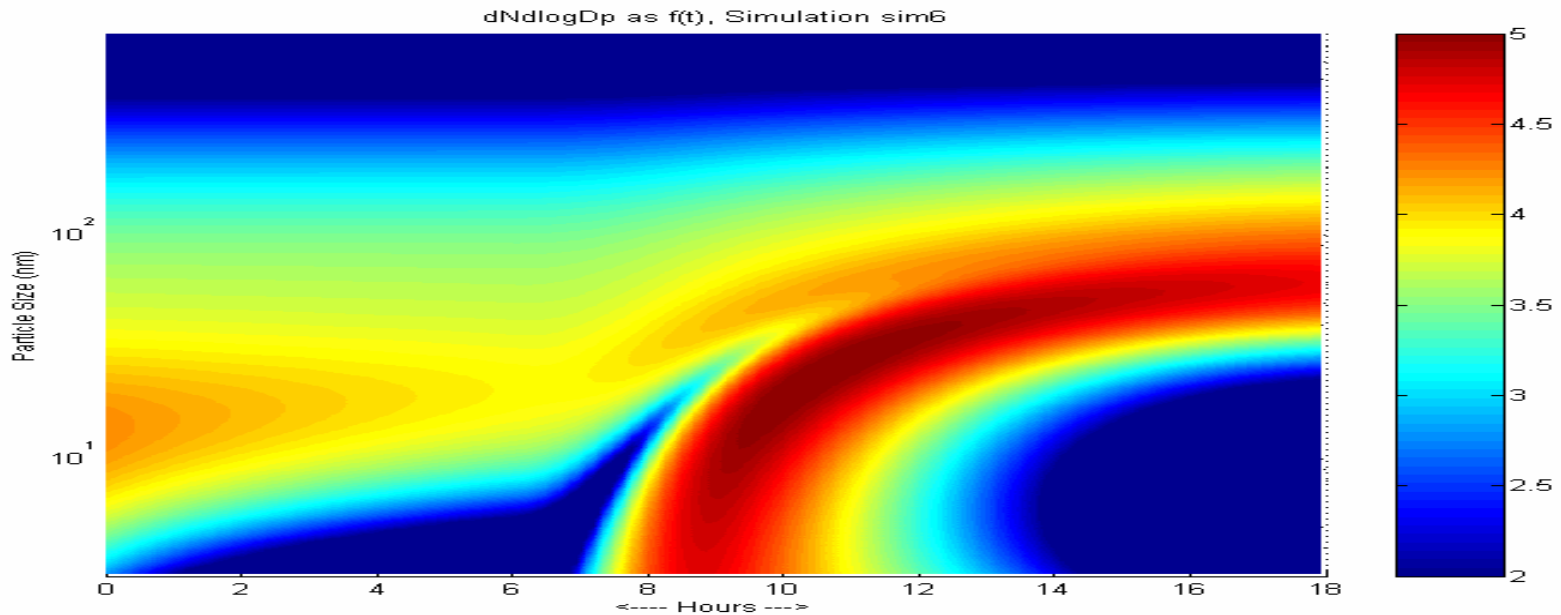


Formation and Growth of Ultrafine PM



July 2, 2001

Preliminary Model Results



- Sulfuric Acid/Water Nucleation and Growth
  - Qualitative behavior OK
  - Cannot predict the days when nucleation happens
- Role of ammonia and organics?
  - Added to the model